Renormalization and Quantum Scaling of Frenkel–Kontorova Models

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Abstract

We generalise the classical Transition by Breaking of Analyticity for the class of Frenkel–Kontorova models studied by Aubry and others to non-zero Planck's constant and temperature. This analysis is based on the study of a renormalization operator for the case of irrational mean spacing using Feynman's functional integral approach. We show how existing classical results extend to the quantum regime. In particular we extend MacKay's renormalization approach for the classical statistical mechanics to deduce scaling of low frequency effects and quantum effects. Our approach extends the phenomenon of hierarchical melting studied by Vallet, Schilling and Aubry to the quantum regime.

Keywords: Transition by breaking of analyticity; renormalization; quantum scaling; specific heat.

1 Introduction

The *Frenkel–Kontorova model* (FK) is a one-dimensional lattice model exhibiting incommensurate structures. It is a system of elastically coupled particles in an external periodic potential (a discrete version of the sine–Gordon model) with Lagrangian

$$L\left(x,\dot{x}\right) = \sum_{n \in \mathbb{Z}} \left\{ \frac{\dot{x}_n^2}{2} - \text{v}\left(x_n, x_{n+1}\right) \right\}, \tag{1}$$

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where

$$v\left(x, x'\right) = \frac{1}{2}\left(x' - x\right)^2 + P\left(x' - x\right) + \frac{u}{4\pi^2}\cos\left(2\pi x\right), \qquad (2)$$

with constants P ("pressure" or $-P$ as tension) and u (amplitude of the onsite potential). We call successive pairs (x_n, x_{n+1}) *bonds* and $v\left(x_n, x_{n+1}\right)$ the *(potential) energy of the bond*. Notice that in (1) and (2) the particles' mass, the elastic coupling strength and the period of the onsite potential are all scaled to one. The FK model is a particular case of the broader class of *(Generalised) Frenkel–Kontorova models* (GFK) with Lagrangian still given by (1) but the bond action v is a generic $\mathcal{C}^2$ function satisfying

$$v\left(x + 1, x' + 1\right) = v\left(x, x'\right)$$
$$\frac{\partial^2 v}{\partial x \partial x'}\left(x, x'\right) \leqslant -C < 0\,.$$

In the space of parameters there are two important limits. In the *integrable* limit, the bond energy, v, depends only on $(x' - x)$. For the FK model (2) the integrable limit is attained at $u = 0$ and its *minimum energy configurations* (i.e. $x \in \mathbb{R}^{\mathbb{Z}}$ such that $\forall M < N, V_{M,N}\left(x\right) \equiv \sum_{n=M}^{N-1} v\left(x_n, x_{n+1}\right)$ is minimum for all variations of x_n with fixed x_M and x_N) are arrays of equally spaced particles with *mean spacing*

$$\rho := \lim_{-M, N \to \infty} \frac{x_N - x_M}{N - M}$$

simply $-P$. In the *anti-integrable* limit [4] the onsite term dominates, which corresponds to $u \to \infty$ in (2). All particles are then in the minima of the potential and the mean spacing is the closest integer to $-P$, or any value in between the two if non-unique.

An interesting set of codimension-2 critical points occur between these two regimes, often called *Transition by Breaking of Analyticity* (TBA): in the space of parameters (u, P), for each irrational ρ there is a curve $P = P_\rho\left(u\right)$ of mean spacing ρ containing a critical value u_c (there may be more than one u_c depending on the potential). The regime for u less than u_c is called *subcritical* (or *sliding phase*) and above u_c *supercritical* (or *pinned phase*) [5]. For the FK model with fixed mean spacing $\rho = \gamma^{-1}$, where $\gamma = \left(1 + \sqrt{5}\right)/2$ is the golden mean, the TBA is at the critical value $u_c \simeq 0.971\,635\,406$ [15]. This is the case most often studied in the literature, since it is presumed to be the highest value of u at which a TBA occurs.

For the case of mean spacing $\rho = \gamma^{-1}$, relabelling the bonds v appropriately [19] as τ and υ results in a Fibonacci sequence of τs and υs where each υ-bond is always surrounded by τ-bonds. The TBA point can be viewed as a fixed point of the renormalization operator that minimises the energy of the sum of successive υ and τ-bonds with suitably chosen space and energy scalings, $\alpha, \mathcal{J} \in \mathbb{R}$

respectively depending on the pair (v, τ) (actually it is also necessary to subtract a constant and a quadratic coboundary but we will suppress reference to these inessential terms) [19]. The renormalization operator has a nontrivial fixed point[1] $(\bar{v}, \bar{\tau})$ with $\alpha \simeq -1.414\,836\,0$ and $\mathcal{J} \simeq 4.399\,143\,9$. This fixed point corresponds to the critical u_c along the curve in (u, P) for $\rho = \gamma^{-1}$, the transition point between the subcritical and supercritical regimes. It has two unstable directions: one along the curve of constant mean spacing, with eigenvalue $\delta \simeq 1.627\,950\,0$ and the other transverse to this curve in the (u, P) plane (which we'll call the P direction), with eigenvalue $\eta = -\mathcal{J}/\gamma \simeq -2.681\,738\,4$ [19, 20].

Whereas the classical ground states of Frenkel–Kontorova models have been extensively studied since the beginning of the 1980's [1, 2, 3, 5, 22] (see also the review in chapter 1 of [11], and the book [10] for several aspects of the FK model), the extension to the quantum regime of the classical Transition by Breaking of Analyticity is still not fully understood. Most of the previous studies stem from the work of Borgonovi *et al.* [8, 9], where the authors do a numerical study of FK model in the supercritical region $u > u_c$ for the case of mean spacing γ^{-1}. They introduce a 'quantum hull function' for the expected positions $\bar{x}_n$ as the extension of Aubry's hull function (see [11], section 1.2) as well as the 'quantum g-function' (which reduces to $\sin(2\pi\bar{x}_n)$ in the classical limit) and verify that by increasing $\hbar$ the quantum hull function becomes a smooth version of the classical hull function and that g_n tends to a sawtooth-like map. Similar results have been later obtained using various numerical or a combination of analytical and numerical methods [6, 7, 17, 16].

In a recent numerical study Zhirov *et al.* [26] claim to observe a 'quantum phase transition' in the FK model at a critical value of Planck's constant between 'sliding phonon gas' and a 'pinned instanton glass'. In fact we expect that due to KAM-type of arguments, for sufficiently irrational mean spacing the phonon energy band will survive for a small perturbation of the integrable limit $u = 0$, where the interactions between phonons of different wavenumber are small. At the anti-integrable limit, on the other hand, when the dominant interaction is the onsite periodic potential, the quantum spectrum consists of N degenerate sets of Bloch bands (N being the total number of particles) whose width is due to tunneling or instanton effects between distinct minima of the onsite potential. As u is decreased from the anti-integrable limit, the degeneracy between Bloch bands corresponding to distinct particles should be lifted, widening the Bloch bands until they merge into a unique phonon band for some non-zero value $u_c(\hbar)$ (possibly not a unique curve).

In addition to the groundstates, it is physically significant to

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[1]This has now been proved by Koch [18] by reformulation as a renormalization on continuous–time Hamiltonian systems and rigorous computer–assisted bounds.

study the effect of the TBA on the low temperature statistical mechanics of FK models. This was done for the classical case in [21]. The quantum statistical mechanics of FK models was considered in a series of papers by Giachetti and Tognetti, e.g. [13, 14], but we are not aware of any work on the effects of the TBA on the quantum statistical mechanics.

The goal of this article is to study the transition above by extending the minimum energy renormalization approach in [19] to non-zero Planck's constant and temperature, which is done in section 2. This is done in a way similar to the classical non-zero temperature extension performed in [21] but requires first an extension of the classical case from ground states to time-periodic solutions. The strategy is to construct a renormalization operator, $\mathcal{R}$, which reduces to the ground state operator, $\mathcal{R}_{cgs}$, when $\hbar$ goes to zero, i.e. $\mathcal{R}|_{\hbar=0} = \mathcal{R}_{cgs}$. Then $(u, P, \ldots, \hbar = 0)$ is an invariant subspace for $\mathcal{R}$ which includes the critical fixed point of renormalization corresponding to the TBA by construction.

In the main section 2 we start by defining a decimation procedure $\oplus$ for pairs of "bond actions" by doing the trace over intermediate particles corresponding to a partial trace over the kernel and the renormalization operator $\mathcal{R}$ by composing the decimation with the appropriate scalings. The quantum eigenvalue κ is also introduced. Next, in subsection 2.1, we show that the classical ground state renormalization, $\mathcal{R}_{cgs}$, is obtained as the limit of zero Planck's constant and frequency of quantum renormalization. In subsection 2.2 the value of the quantum eigenvalue is determined by analysing the linearised or phonon problem. Finally in section 2.4 the results obtained are 'Wick rotated' to obtain the scaling laws for quantum thermal quantities, and an extension of the phenomenon of hierarchical melting studied by Vallet, Schilling and Aubry [24, 23, 25] to the quantum regime is proposed.

2   Renormalization and scaling

We begin by introducing the renormalization procedure for the action of time-periodic functions of prescribed period. Consider the class of models with the following formal sum for the action

$$\mathcal{S}(x; T) = \sum_{n \in \mathbb{Z}} s(x_n, x_{n+1}; T).$$

for time–periodic functions x_n of period T, where the *bond action s* is given by

$$s(x, x'; T) = \int_0^T \left\{ \frac{\dot{x}^2}{2} - \mathrm{v}(x, x') \right\} dt, \tag{3}$$

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and v is a GFK bond potential energy. The quantum renormalization will concern the trace of the kernel which is

$$K'(T, \hbar) = \int \mathcal{D}'x \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{S}(x;T)},$$

where the notation $\mathcal{D}'x$ means that the integration is to be performed over the space of periodic paths x with period T and includes the integration over the endpoints $dx(0)$ (i.e. $x(T) = x(0)$ and $\mathcal{D}'x = dx(0)\,\mathcal{D}x$). Rescaling time $t \to t/T$ and defining $\Omega = 2\pi/T$ the bond action can be rewritten as

$$s\left(x, x'; \frac{2\pi}{\Omega}\right) = \frac{2\pi}{\Omega} \int_0^1 \left\{ \frac{\Omega^2}{8\pi^2}\dot{x}^2 - \mathrm{v}(x, x') \right\} dt, \qquad (4)$$

and now s acts on the space of period-one functions $x, x' : \mathbb{R}/\mathbb{Z} \to \mathbb{R}$ or *loops*.

Now let $\mathrm{x} \in \mathbb{R}^{\mathbb{Z}}$ be a classical ground state and call a bond action s a τ or an υ as for the renormalization for classical ground states in [19]. For the case of mean spacing γ^{-1} the sequence of bond actions then forms an infinite Fibonacci sequence of τ and υ types of bonds where each υ is always surrounded by τs. At this point one wants to eliminate all particles z from sequences of the form $\upsilon(x, z; \Omega) + \tau(z, x'; \Omega)$ (for simplicity we use Ω as an argument of action bonds instead of $2\pi/\Omega$ from now on). In order to do this define the following decimation operator $\oplus$ acting on pairs of bond actions (υ, τ) as

$$(\upsilon \oplus \tau)(x, x'; \Omega) = -\mathrm{i}\hbar \ln \int \mathcal{D}'z \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left[\upsilon(x,z;\Omega)+\tau\left(z,x';\Omega\right)\right]}. \qquad (5)$$

The decimated functional $\upsilon \oplus \tau$ still has the form of an action bond in the sense that it acts on pairs of loops (x, x'). The renormalization operator is defined as the composition of a decimation and scalings as

$$\mathcal{R}\left[\begin{array}{c} \tau(x, x'; \Omega) \\ \upsilon(x, x'; \Omega) \end{array}\right] = \frac{\mathcal{J}}{\varepsilon}\left[\begin{array}{c} (\upsilon \oplus \tau)(x/\alpha, x'/\alpha; \Omega/\varepsilon) \\ \tau(x/\alpha, x'/\alpha; \Omega/\varepsilon) \end{array}\right], \qquad (6)$$

which includes a scaling of frequencies, ε, still undetermined at this point. The global scaling of bond actions is $\mathcal{J}/\varepsilon$ instead of just $\mathcal{J}$ because the renormalization now acts on actions instead of energies as in the classical ground state case. By performing the composition of (6) and (5) explicitly one can see that the natural scale factor $\kappa = \mathcal{J}/\varepsilon$ for Planck's constant arises and $\mathcal{R}$ can be seen as acting on the extended space of $(\tau, \upsilon, \hbar)$ for $\hbar \geq 0$ as

$$\mathcal{R}: \left\{ \begin{array}{l} \tilde{\tau}(x, x'; \Omega) = -\mathrm{i}\kappa\hbar \int \mathcal{D}'z \, \mathrm{e}^{\frac{\mathrm{i}}{\kappa\hbar}\frac{\mathcal{J}}{\varepsilon}\left\{\upsilon(x/\alpha,z;\Omega/\varepsilon)+\tau\left(z,x'/\alpha;\Omega/\varepsilon\right)\right\}} \\ \tilde{\upsilon}(x, x'; \Omega) = \frac{\mathcal{J}}{\varepsilon}\tau(x/\alpha, x'/\alpha; \Omega/\varepsilon) \\ \tilde{\hbar} = \kappa\hbar \end{array} \right. .$$

$$(7)$$

We interpret κ as the eigenvalue of $\mathcal{R}$ in the direction of Planck's constant.

2.1 Semiclassical approximation and ground state limit

As a first step to connect the quantum renormalization (6) with the ground state renormalization of [19], one can look at the decimation operator (5) in the stationary phase approximation for small $\hbar$:

$$(v \oplus \tau)\left(x, x'; \Omega\right) = -i\hbar \ln \int \mathcal{D}'z\, \delta\left(z - z_{\text{cl.}}\left(x, x'; \Omega\right)\right) \times$$
$$\times e^{\frac{i}{\hbar}\left\{v(x,z;\Omega)+\tau\left(z,x';\Omega\right)\right\}}. \qquad (8)$$

Here $z_{\text{cl.}}\left(x, x'; \Omega\right)$ is the classical path of period one satisfying the Euler–Lagrange equations

$$\left.\frac{\delta\left[v\left(x, z; \Omega\right) + \tau\left(z, x'; \Omega\right)\right]}{\delta z}\right|_{z=z_{\text{cl.}}\left(x,x';\Omega\right)} = 0. \qquad (9)$$

In the classical limit one is thus left with a dynamical problem (9) and the decimated action (8) can be rewritten as

$$\underset{z \in \text{loops}}{\text{sta}}\left[v\left(x, z; \Omega\right) + \tau\left(z, x'; \Omega\right)\right], \qquad (10)$$

the sum of bond actions evaluated at $z = z_{\text{cl.}}$, given by (9), which stationarises the sum $v+\tau$ over the space of all loops $\{z : \mathbb{R}/\mathbb{Z} \to \mathbb{R}\}$.

2.1.1 Ground state limit

The ground state decimation can now be taken as the limit $\Omega \to 0$ of (8) or (10). To see this, notice that in this limit only the classical ground states contribute to the kernel and

$$\int \mathcal{D}'z\, e^{\frac{i}{\hbar}\left\{v(x,z)+\tau\left(z,x'\right)\right\}} \simeq e^{-\frac{2\pi i}{\hbar\Omega}\left\{v^{(v)}(x,z)+v^{(\tau)}\left(z,x'\right)\right\}},$$

where (x, z, x') is a segment of a classical ground state and $z\left(x, x'\right)$ minimises the sum $v + \tau$. Taking the logarithm and multiplying by $-i\hbar$, this results in the decimation (5) being

$$(v \oplus \tau)\left(x, x'; 0\right) = \lim_{\Omega \to 0} -\frac{2\pi}{\Omega}\min_{z \in \mathbb{R}}\left[v^{(v)}\left(x, z\right) + v^{(\tau)}\left(z, x'\right)\right] \qquad (11)$$

(the factor $2\pi/\Omega$ is kept in the above expression simply to control the divergence of decimation). Apart from the limit factor

$\lim_{\Omega \to 0} -2\pi/\Omega$ this is in fact the classical ground state decimation in [19] and so the renormalization (6) becomes

$$
\mathcal{R} \left[\begin{array}{c} \tau\left(x, x'; 0\right) \\ \upsilon\left(x, x'; 0\right) \end{array} \right] \quad \simeq \quad \lim_{\Omega \to 0} \left[\begin{array}{c} -\frac{2\pi}{\Omega} \mathcal{J} \left(\mathrm{v}^{(\upsilon)} \oplus_{\mathrm{cgs}} \mathrm{v}^{(\tau)} \right) \left(\mathrm{x}/\alpha, \mathrm{x}'/\alpha\right) \\ -\frac{2\pi}{\Omega} \mathcal{J} \mathrm{v}^{(\tau)} \left(\mathrm{x}/\alpha, \mathrm{x}'/\alpha\right) \end{array} \right]
$$

$$
= \quad \lim_{\Omega \to 0} -\frac{2\pi}{\Omega} \mathcal{R}_{\mathrm{cgs}} \left[\begin{array}{c} \mathrm{v}^{(\tau)}\left(\mathrm{x}, \mathrm{x}'\right) \\ \mathrm{v}^{(\upsilon)}\left(\mathrm{x}, \mathrm{x}'\right) \end{array} \right], \tag{12}
$$

where $\oplus_{\mathrm{cgs}}$ and $\mathcal{R}_{\mathrm{cgs}}$ are the decimation and renormalization operators for the classical ground states, and $\varepsilon \in \mathbb{R}$ is still undetermined at this point. The renormalization $\mathcal{R}$ has therefore a fixed point (the TBA fixed point), with ground states of mean spacing $\rho = \gamma^{-1}$, in the $\Omega = 0$ subspace consisting of

$$
\left[\begin{array}{c} \bar{\tau}\left(x, x'; 0\right) \\ \bar{\upsilon}\left(x, x'; 0\right) \end{array} \right] = \lim_{\Omega \to 0} -\frac{2\pi}{\Omega} \left[\begin{array}{c} \bar{\mathrm{v}}^{(\tau)}\left(x, x'\right) \\ \bar{\mathrm{v}}^{(\upsilon)}\left(x, x'\right) \end{array} \right],
$$

where $(\bar{\mathrm{v}}^\tau, \bar{\mathrm{v}}^\upsilon)$ is the fixed point of the ground state renormalization operator $\mathcal{R}_{\mathrm{cgs}}$, because applying expression (12) at the TBA fixed point results in

$$
\mathcal{R} \left[\begin{array}{c} \bar{\tau}\left(x, x'; 0\right) \\ \bar{\upsilon}\left(x, x'; 0\right) \end{array} \right] = \lim_{\Omega \to 0} -\frac{2\pi}{\Omega} \left[\begin{array}{c} \bar{\mathrm{v}}^{(\tau)}\left(\mathrm{x}, \mathrm{x}'\right) \\ \bar{\mathrm{v}}^{(\upsilon)}\left(\mathrm{x}, \mathrm{x}'\right) \end{array} \right] = \left[\begin{array}{c} \bar{\tau}\left(x, x'; 0\right) \\ \bar{\upsilon}\left(x, x'; 0\right) \end{array} \right].
$$

2.2 Renormalization for the phonon spectrum

Close to the ground state, for small Ω^2, the relevant contributions are approximately given by the normal modes or *phonons*. For a GFK model at irrational mean spacing ground state, ρ, the phonon spectrum includes zero in the subcritical regime, but the minimum frequency or *phonon gap* is positive above the critical point u_c [5]. The phonon contribution to the trace of the kernel is given by doing a quadratic approximation which is (with $x_n = \mathrm{x}_n + \xi_n$)

$$
K'\left(\mathrm{x}, \frac{2\pi}{\Omega}\right) \quad \simeq \quad \mathrm{e}^{-\frac{2\pi \mathrm{i}}{\hbar \Omega} \sum_n \mathrm{v}^{(n)}\left(\mathrm{x}_n, \mathrm{x}_{n+1}\right)} \times \tag{13}
$$

$$
\times \quad \int \mathcal{D}'\xi \, \mathrm{e}^{\frac{\pi \mathrm{i}}{\hbar \Omega} \sum_n \int_0^1 \left\{ \frac{\Omega^2}{4\pi^2} m^{(n)}\left(\dot{\xi}_n, \dot{\xi}_{n+1}\right) - u^{(n)}\left(\xi_n, \xi_{n+1}\right) \right\} dt},
$$

where the kinetic term was generalised to a symmetric quadratic form in the velocities

$$
m^{(n)}\left(\dot{\xi}, \dot{\xi}'\right) = m_{11}^{(n)} \dot{\xi}^2 + 2 m_{12}^{(n)} \dot{\xi} \dot{\xi}' + m_{22}^{(n)} \dot{\xi}'^2
$$

(as will become clear later on the renormalization operator introduces coupling between the velocities of neighbouring particles), and u is also a symmetric quadratic form

$$
u^{(n)}\left(\xi, \xi'\right) = u_{22}^{(n)} \xi^2 - 2 u_{12}^{(n)} \xi \xi' + u_{11}^{(n)} \xi'^2.
$$

The first term in (13) is simply the classical ground state and corresponds to (12), so one wants to apply the decimation (5) to the sum of the quadratic parts of bond actions of the form

$$\frac{\pi}{\Omega} \left\{ \frac{\Omega^2}{4\pi^2} \left[m^{(v)} \left(\dot{\xi}, \dot{\zeta} \right) + m^{(\tau)} \left(\dot{\zeta}, \dot{\xi}' \right) \right] - \left[u^{(v)} \left(\xi, \zeta \right) + u^{(\tau)} \left(\zeta, \xi' \right) \right] \right\}.$$

Because this sum is quadratic in the particle to eliminate, ζ, the corresponding functional integral can be calculated (for example by Gaussian integration of the Fourier transformed sum of action bonds [27]) and the semiclassical approximation is exact in this case. To first order in Ω^2 the result is[2]

$$e^{\frac{i\pi}{\hbar\Omega} \left\{ \frac{\Omega^2}{4\pi^2} \left[m^{(v)} \left(\dot{\xi}, \dot{\zeta} \right) + m^{(\tau)} \left(\dot{\zeta}, \dot{\xi}' \right) \right] - \left[u^{(v)} (\xi, \zeta) + u^{(\tau)} (\zeta, \xi') \right] \right\}} \simeq$$

$$\simeq e^{\frac{i\pi}{\hbar\Omega} \left\{ \frac{\Omega^2}{4\pi^2} \tilde{m}^{(\tau)} \left(\dot{\xi}, \dot{\xi}' \right) - \tilde{u}^{(\tau)} \left(\xi, \xi' \right) \right\}},$$

where $\tilde{m}^{(\tau)}$ is a new symmetric quadratic form with components given by

$$\tilde{m}_{11}^{(\tau)} = m_{11}^{(v)} + \frac{2 m_{12}^{(v)} u_{12}^{(v)}}{u_{22}^{(v)} + u_{11}^{(\tau)}} + \frac{\left(m_{22}^{(v)} + m_{11}^{(\tau)} \right) u_{12}^{(v)2}}{\left(u_{22}^{(v)} + u_{11}^{(\tau)} \right)^2}$$

$$\tilde{m}_{12}^{(\tau)} = \frac{m_{12}^{(v)} u_{12}^{(\tau)} + m_{12}^{(\tau)} u_{12}^{(v)}}{u_{22}^{(v)} + u_{11}^{(\tau)}} + \frac{\left(m_{22}^{(v)} + m_{11}^{(\tau)} \right) u_{12}^{(v)} u_{12}^{(\tau)}}{\left(u_{22}^{(v)} + u_{11}^{(\tau)} \right)^2} \quad (14)$$

$$\tilde{m}_{22}^{(\tau)} = m_{22}^{(\tau)} + \frac{2 m_{12}^{(\tau)} u_{12}^{(\tau)}}{u_{22}^{(v)} + u_{11}^{(\tau)}} + \frac{\left(m_{22}^{(v)} + m_{11}^{(\tau)} \right) u_{12}^{(\tau)2}}{\left(u_{22}^{(v)} + u_{11}^{(\tau)} \right)^2}$$

and the new form $\tilde{u}^{(\tau)}$ has components

$$\tilde{u}_{11}^{(\tau)} = u_{11}^{(v)} - \frac{u_{12}^{(v)2}}{u_{22}^{(v)} + u_{11}^{(\tau)}}$$

$$\tilde{u}_{12}^{(\tau)} = \frac{u_{12}^{(v)} u_{12}^{(\tau)}}{u_{22}^{(v)} + u_{11}^{(\tau)}} \quad (15)$$

$$\tilde{u}_{22}^{(\tau)} = u_{22}^{(\tau)} - \frac{u_{12}^{(\tau)2}}{u_{22}^{(v)} + u_{11}^{(\tau)}}.$$

With these new quadratic forms, the decimation (5) becomes simply

$$(v \oplus \tau) \left(x, x'; \Omega \right) = \text{(c.g.s. decimation)} + \quad (16)$$

$$+ \frac{1}{\Omega} \int_0^1 \Omega^2 \tilde{m}^{(\tau)} \left(\xi, \xi' \right) - \tilde{u}^{(\tau)} \left(\xi, \xi' \right) \, dt,$$

[2]There is possibly also a logarithmic term due to the integration measure which corresponds to a redefinition of the ground state energy.

where 'c.g.s decimation' is the decimation (11). For the renormalization (6) one also needs the 'undecimated' bond actions which correspond to isolated bond actions of type τ, so one should define also

$$
\begin{aligned}
\tilde{m}^{(v)}\left(\xi, \xi'\right) &= m^{(\tau)}\left(\xi, \xi'\right) \\
\tilde{u}^{(v)}\left(\xi, \xi'\right) &= u^{(\tau)}\left(\xi, \xi'\right).
\end{aligned}
\tag{17}
$$

For a GFK model (3) at the start of renormalization, for either type τ or v of bonds the quadratic forms are $m_{12} = 0$, $m_{11} + m_{22} = 1$, $u_{jj} = v_{,jj}\left(\mathrm{x}, \mathrm{x}'\right)$ for $j = 1, 2$ and $u_{12} = -v_{,12}\left(\mathrm{x}, \mathrm{x}'\right)$, where the subscripts in v denote differentiation with respect to the first and second variables and $\left(\mathrm{x}, \mathrm{x}'\right)$ is a segment of a classical ground state. Because u is then dependent on $\left(\mathrm{x}, \mathrm{x}'\right)$, after iterating the above transformations (14), (15) and (17) one ends up with a set of asymptotic quadratic forms depending on the ground state, $\bar{m}_{\mathrm{x},\mathrm{x}'}^{(\tau)}$, $\bar{m}_{\mathrm{x},\mathrm{x}'}^{(v)}$, $\bar{u}_{\mathrm{x},\mathrm{x}'}^{(\tau)}$ and $\bar{u}_{\mathrm{x},\mathrm{x}'}^{(v)}$ which scale by factors[3] $\omega = \alpha^2 \varepsilon^2 / \mathcal{J} \simeq 1.255\,071$ for the mass forms and $\mathcal{J}/\alpha^2$ for the potential forms [19], i.e.

$$
\left\{
\begin{aligned}
\tilde{\bar{m}}_{\mathrm{x},\mathrm{x}'}^{(\tau)} &\simeq \frac{\alpha^2 \varepsilon^2}{\mathcal{J}} \bar{m}_{\mathrm{x},\mathrm{x}'}^{(\tau)} \\
\tilde{\bar{m}}_{\mathrm{x},\mathrm{x}'}^{(v)} &\simeq \frac{\alpha^2 \varepsilon^2}{\mathcal{J}} \bar{m}_{\mathrm{x},\mathrm{x}'}^{(\tau)} \\
\tilde{\bar{u}}_{\mathrm{x},\mathrm{x}'}^{(\tau)} &\simeq \frac{\alpha^2}{\mathcal{J}} \bar{u}_{\mathrm{x},\mathrm{x}'}^{(\tau)} \\
\tilde{\bar{u}}_{\mathrm{x},\mathrm{x}'}^{(v)} &\simeq \frac{\alpha^2}{\mathcal{J}} \bar{u}_{\mathrm{x},\mathrm{x}'}^{(v)}
\end{aligned}
\right. .
\tag{18}
$$

Finally, using (14–18), and defining

$$
\begin{aligned}
\bar{\tau}\left(x, x'; \Omega\right) &:= \frac{\pi}{\Omega}\Bigg[-\bar{\mathrm{v}}^{(\tau)}\left(\mathrm{x}, \mathrm{x}'\right) \\
&+ \int_0^1 \left\{\frac{\Omega^2}{4\pi^2}\bar{m}_{\mathrm{x},\mathrm{x}'}^{(\tau)}\left(\xi, \xi'\right) - \bar{u}_{\mathrm{x},\mathrm{x}'}^{(\tau)}\left(\xi, \xi'\right)\right\} dt\Bigg] \\
\bar{v}\left(x, x'; \Omega\right) &:= \frac{\pi}{\Omega}\Bigg[-\bar{\mathrm{v}}^{(v)}\left(\mathrm{x}, \mathrm{x}'\right) \\
&+ \int_0^1 \left\{\frac{\Omega^2}{4\pi^2}\bar{m}_{\mathrm{x},\mathrm{x}'}^{(\tau)}\left(\xi, \xi'\right) - \bar{u}_{\mathrm{x},\mathrm{x}'}^{(\tau)}\left(\xi, \xi'\right)\right\} dt\Bigg],
\end{aligned}
$$

the renormalization (7) at $\left(\bar{\tau}, \bar{v}, \hbar\right)$ becomes

$$
\mathcal{R}\left[\begin{array}{c} \bar{\tau}\left(x, x'; \Omega\right) \\ \bar{v}\left(x, x'; \Omega\right) \\ \hbar \end{array}\right] \simeq \left[\begin{array}{c} \bar{\tau}\left(x, x'; \Omega\right) \\ \bar{v}\left(x, x'; \Omega\right) \\ \kappa\hbar \end{array}\right].
$$

Thus, by including the scaling of frequencies $\varepsilon \simeq 1.649\,415$ (see footnote 3) in the renormalization (6), the point $\left(\bar{\tau}, \bar{v}, 0\right)$ becomes an

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[3] In [19] the scaling is actually for the quantities $a_n := u_{22}^{(n-1)} + u_{11}^{(n)}$, $b_n := u_{12}^{(n)}$, $c_n := m_{22}^{(n-1)} + m_{11}^{(n)}$ and $d_n := m_{12}^{(n)}$ with scaling constants $\omega \simeq 1.255\,071$ for a_n and b_n and β/α for c_n and d_n, so the first and third equations in (18) are defined up to a quadratic coboundary. Here we use the scale factors for frequency $\varepsilon := \sqrt{\omega \mathcal{J}/\alpha^2} \simeq 1.649\,415$ and energy $\mathcal{J} = \alpha\beta$ instead. The origin of ω is still a mystery.

approximate fixed point for small Ω (actually a line of fixed points parametrised by Ω). In particular the phonon spectrum is asymptotically self-similar under scaling by ε in the direction of Ω.

Finally, note that fixing ε also determines the eigenvalue in the $\hbar$-direction[4] as $\kappa = \mathcal{J}/\varepsilon \simeq 2.630\,716$.

2.3 Scaling of the kernel

The results above imply that the effect of including both the frequencies and quantum directions, close to the TBA fixed point (for $\Delta u := u - u_c$, $\Delta P := P - P_{\gamma^{-1}}(u_c)$, Ω and $\hbar$ small), is that the following asymptotic relation of bond actions (regarded as functions in parameter space) holds

$$(\tau, \upsilon)(\Delta u, \Delta P, \Omega, \hbar) \simeq \frac{\mathcal{J}}{\varepsilon}(\tau, \upsilon)(\delta \Delta u, \eta \Delta P, \varepsilon \Omega, \kappa \hbar). \qquad (19)$$

If K'_{J,F_m} is the trace of the kernel for a chain of size F_m, the mth Fibonacci number, in the discretised form with J 'time steps' (such that $K'_{F_m} = \lim_{J \to \infty} K'_{J,F_m}$), then

$$K'_{J,F_m}(\Delta u, \Delta P, \Omega, \hbar) \simeq K'_{J,F_{m-1}}(\delta \Delta u, \eta \Delta P, \varepsilon \Omega, \kappa \hbar) \left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right)^{JF_{m-1}}.$$

Here the multiplying factor comes from the functional integration measure due to the change of coordinates (here with diagonal mass components $\mu^{(n)} = \bar{m}_{22}^{(n-1)} + \bar{m}_{11}^{(n)}$)

$$\prod_n \left(\mathcal{D}'_J \frac{x_n}{\alpha}\right)(\Omega, \hbar) = \prod_n \prod_{j=0}^{J-1} \sqrt{\frac{\mu^{(n)}\Omega J}{4\pi^2 i\,\hbar}}\, \frac{dx_n^{(j)}}{|\alpha|}$$

$$= \prod_n \left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right)^J (\mathcal{D}'_J \tilde{x}_n)(\varepsilon\Omega, \kappa\hbar),$$

where $\tilde{x}_n$ are the positions of the renormalized particles.

2.4 Non-zero temperature scaling

The quantum partition function at temperature Θ can be easily obtained from the trace of the kernel by Wick rotation, i.e. doing $2\pi/\Omega = -i\beta\hbar$, where $\beta = 1/\Theta$. The quantum partition function is then

$$\mathcal{Z}(\beta\hbar, \hbar) = K'(-i\beta\hbar, \hbar) = \int \mathcal{D}'x\, e^{-\beta\mathcal{S}_E(x;\beta\hbar)},$$

---

[4]This result was published in [12] containing a mistake: $k = \mathcal{J}\varepsilon$ instead of the correct value $\kappa = \mathcal{J}/\varepsilon$.

where the *Euclidean action* for the FK model is

$$
\begin{aligned}
\mathcal{S}_E &= \sum_n s_E\left(x_n, x_{n+1}; \beta\hbar\right) \\
&= \sum_n \int_0^1 \left\{ \frac{\dot{x}_n^2}{2\left(\beta\hbar\right)^2} + \mathrm{v}\left(x_n, x_{n+1}\right) \right\} dt_E,
\end{aligned}
$$

and the integration is now over the rescaled Euclidean time $t_E \in \mathbb{R}/\mathbb{Z}$. Comparing with (4), the *Euclidean bond action* s_E can be written as

$$
s_E\left(x, x'; \beta\hbar\right) = \left[-\frac{\Omega}{2\pi}\, s\left(x, x'; \Omega\right) \right]_{\Omega = 2\pi \mathrm{i}/\beta\hbar},
$$

and has units of an energy instead of an action because of the multiplying factor $\Omega/2\pi$. This gives another direction to which renormalization can be extended, the temperature direction $\Theta = 1/\beta$. Define then the operator $\oplus_E$ by 'Wick rotating' the operator $\oplus$ for the trace of the kernel (5), to obtain

$$
\left(\upsilon_E \oplus_E \tau_E\right)\left(x, x'; \beta\hbar\right) = -\beta^{-1} \ln \int \mathcal{D}'z\, \mathrm{e}^{-\beta\left[\upsilon_E(x, z; \beta\hbar) + \tau_E\left(z, x'; \beta\hbar\right)\right]},
$$

and the renormalization as

$$
\mathcal{R}_E \left[\begin{array}{c} \tau_E\left(x, x'; \beta\hbar\right) \\ \upsilon_E\left(x, x'; \beta\hbar\right) \end{array} \right] = \left[\begin{array}{c} \mathcal{J}\tau_E\left(x/\alpha, x'/\alpha; \varepsilon\beta\hbar\right) \\ \mathcal{J}\upsilon_E\left(x/\alpha, x'/\alpha; \varepsilon\beta\hbar\right) \end{array} \right].
$$

Therefore, close to the TBA fixed point the renormalization operator leads to the corresponding relation to (19) for Euclidean bond actions:

$$
\left(\tau_E, \upsilon_E\right)\left(\Delta u, \Delta P, \beta\hbar, \hbar\right) \simeq \mathcal{J}\left(\tau_E, \upsilon_E\right)\left(\delta\Delta u, \eta\Delta P, \varepsilon^{-1}\beta\hbar, \kappa\hbar\right),
$$

so under the renormalization $\mathcal{R}_E$ there is a fixed point at $\hbar = 0$, $\beta\hbar = \infty$, with an unstable eigenvalue of $\kappa\varepsilon = \mathcal{J} \simeq 4.339\,143\,9$ in the temperature direction. Although this agrees with the scaling of [21] for classical statistical mechanics, the result here includes the momentum contribution and corresponds to the quantum correction of the low temperature classical result, in the region $\Theta \ll \hbar$ in which the classical partition function is not valid (see [11], section 3.2). Denoting by $\mathcal{Z}_{F_m}\left(\Delta u, \Delta P, \Theta, \hbar\right)$ the quantum partition function for a chain of F_m particles at temperature Θ, regarded as a function in parameter space, the renormalization picture leads to

$$
\mathcal{Z}_{F_m}\left(\Delta u, \Delta P, \Theta, \hbar\right) \simeq \mathcal{Z}_{F_{m-1}}\left(\delta\,\Delta u, \eta\,\Delta P, \mathcal{J}\,\Theta, \kappa\,\hbar\right)\left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\,\varepsilon}\right)^{JF_{m-1}}.
$$

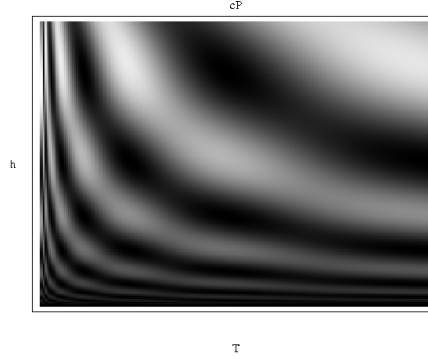The free energy $f = -\Theta \lim_{m \to \infty} \ln \mathcal{Z}_{F_m}/F_m$ therefore behaves like

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Figure 1: Example of the behaviour of c_P for the choice of $k(a,b) = [c^+ k^+(a,b) + c^- k^-(a,b)]\, e^{-c\left(\frac{a}{\ln \mathcal{J}} - \frac{b}{\ln \kappa}\right)}$ in equation (21) with $c = 1/2$, $c^+ = 1$, $c^- = 1/5$ and $k^\pm = 1 + \cos 2\pi \left(\frac{a}{\ln \mathcal{J}} \pm \frac{b}{\ln \kappa}\right)$.

(using $\gamma^{-1} = \lim_{m \to \infty} F_{m-1}/F_m$)

$$f(\Delta u, \Delta P, \Theta, \hbar) \simeq \frac{1}{\gamma \mathcal{J}} f(\delta\, \Delta u, \eta\, \Delta P, \mathcal{J}\, \Theta, \kappa\, \hbar) - \frac{\Theta J}{\gamma} \ln\left(\frac{\sqrt{\mathcal{J}}}{|\alpha|\, \varepsilon}\right),$$

close to the TBA fixed point, and $e = -\Theta^2\, \partial(f/\Theta)/\partial\Theta$, the energy per particle, like

$$e(\Delta u, \Delta P, \Theta, \hbar) \simeq \frac{1}{\gamma \mathcal{J}} e(\delta\, \Delta u, \eta\, \Delta P, \mathcal{J}\, \Theta, \kappa\, \hbar).$$

This leads to the following scaling law for the specific heat per particle at constant pressure $c_P = \partial e/\partial\Theta$:

$$c_P(\Delta u, \Delta P, \Theta, \hbar) \simeq \gamma^{-1} c_P(\delta\, \Delta u, \eta\, \Delta P, \mathcal{J}\, \Theta, \kappa\, \hbar). \qquad (20)$$

In particular close to the TBA, with $\Delta u = \Delta P = 0$ for small Θ and $\hbar$, equation (20) suggests that in the $(\Theta, \hbar)$-plane the specific heat shows a sequence of modulated ridges, which are invariant under scaling by $(\mathcal{J}, \kappa)$:

$$c_P(\Theta, \hbar) \simeq \Theta^{\frac{\ln \gamma}{\ln \mathcal{J}}}\, k(\ln \Theta, \ln \hbar), \qquad (21)$$

with $k(a + \ln \mathcal{J}, b + \ln \kappa) = k(a,b)$, for all a and b (see figure 1). These ridges thus constitute the extension to the $(\Theta, \hbar)$-plane of the sequence of *Schottky anomalies* responsible for the phenomenon of *hierarchical melting* of the chain [24, 23, 25].

Acknowledgements

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